

Ethyl hydroperoxide  
3031-74-1 | DTXSID70184402

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -75.6 °C

Global applicability domain: Inside

Local applicability domain index: 5.06e-01

Confidence level: 4.56e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethyl hydroperoxide</div> <div>Measured: -100</div> <div>Predicted: -75.6</div>	<div>Image not found</div> <div>Methanol</div> <div>Measured: -97.6</div> <div>Predicted: -93.5</div>	<div>Image not found</div> <div>Peracetic acid</div> <div>Measured: -0.200</div> <div>Predicted: 5.24</div>
<div>Image not found</div> <div>tert-Butyl hydroperoxide</div> <div>Measured: -8.00</div> <div>Predicted: -23.0</div>	<div>Image not found</div> <div>Acetaldehyde, hydroxy-</div> <div>Measured: 97.0</div> <div>Predicted: 63.2</div>	